Crystal, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture no. 20 d 3D Point Groups XII: Classification of Point Groups into 7 Crystal Systems

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Classification of Point Groups into 7 Crystal Sy 7 Crystal Systems Characteristic Point Groups Symmetry Triclinic

So, in the previous videos, we developed 32 3 dimensional point groups. Now, there are different ways of classifying these point groups into different classes, one very common classification is the 7 crystal systems. So, 7 crystal systems are nothing but 7 different types of point group and what is used as a basis for this classification. So, 7 crystal systems so 32 point groups will be classified into 7 crystal systems and the basis for classification is the characteristic symmetry that is point groups having certain symmetry will be put into certain crystal systems.

So, we will do it and this one by one for the 7 critical systems let us start with the names of the crystal system, the first system we will list is Triclinic and the characteristic symmetry for that is either a 1 fold axis which actually means no symmetry. So, if a crystal has no rotational symmetry the point group has no rotational symmetry, it will be having a 1 fold axis or if it has just a center of inversion 1 bar.

So, any point group having 1 or 1 bar as its symmetry operation will be considered and nothing more, nothing beyond this, because, you know, there are a lot of when we develop there were a lot of point groups, which were having the center of inversion. So, we will not consider all of them as triclinic we will consider the one's which are triclinic is which has only 1 bar as a symmetry operation and nothing else.

So, either no symmetry or 1 bar symmetry. So, you can see from this that there are only 2 point groups which we developed with the qualify 1 or in the Schoenflies notation C 1 or 1 bar which is in the Schoenflies notation H C i i for inversion center.

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4m2 (D2d), 4mm (D4h)

The second crystal system is monoclinic here the characteristics symmetry is 2 or 2 bar and you are now well familiar the 2 bar is nothing but a mirror plane. So, the point groups which will which will belong to the monoclinic system will be 2 or C 2 m or C s and 2 by m which is C 2h 2 fold with a horizontal mirror that is the Schoenflies notation C 2h then we come to the third crystal system orthorhombic, orthorhombic requires 3 perpendiculars 2 folds 3 perpendicular 2 folds or 2 bar point groups which will belong to this crystal system.

The dihedral group 2 2 2 the Schoenflies notation D 2 or mm2 which is C 2V or finally mmm. So, this as 3 orthogonal mirrors as well as 3 orthogonal 2 fold in Schoenflies notation, D 2h.

Let us come to the tetragonal point to, tetragonal crystal system. Here the requirement of symmetry is one 4 or 4 bar access. So the point groups will be 4 obviously will qualify 4 bar will also qualify 4 bar Schoenflies notations 4 then you have the dihedral group 4 2 2 then you have 4 fold with vertical mirrors 4 mm C 4v in Schoenflies, v indicating the vertical mirror with the 4 fold axis you have 4 by m C 4h for horizontal mirror 4 bar m 2 Schoenflies

notation D 2d, d for diagonal mirror diagonal mirror with the dihedral point group 2 2 2 D 2d. And finally, 4 by m mm which is D 4h.

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 $4mm(C_{4v}), \frac{4}{m}(C_{4h}),$ $\frac{7}{4}m2(D_{2d}), \frac{4}{m}mm(D_{4h})$ Trigonal One 3 3, 3, 32, 5m, 3m $(C_3, C_{3t}, D_3, C_{3v}, D_{3d})$ Hexagonal One 6 or $\overline{6}$ 6 (C₆), $\overline{6}$ (C_{3h}), 622 (D₆) 6mm (C_{6V}), $\frac{6}{m}$ (C_{6h}), $\overline{6}m2$ (D_{3h}), $\frac{6}{m}mm$ (D_{6h})

So, you can see that 7 point groups belong to the tetragonal crystal system then we come to the trigonal system which is characterized by one 3 fold axis to the point groups which will belong to this will be 3, 3 bar, 32, 3m 3 bar m. The corresponding Schoenflies notations are C 3, 3 bar is C 3 i let me write it let me not use brackets C 3 C 3 i, 32 is D 3 the dihedral group 3 m is C 3v, 3 bar m is D 3d.

Hexagonal characteristic symmetry one 6 or 6 bar we had 6 which is the C 6, 6 bar which is C 3h note that the 6 bar axis is a 3 fold axis with a horizontal mirror. So, that is what is reflected in the Schoenflies designation 622, the dihedral group D 6, 6 mm C 6v 6 by m C 6 h 6 bar m2 D 3h 6 by m mm D 6h.

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Une 0 0, 0, 02, 011, 011 irigmai (C3, C31, D3, C3v, D3d) Hexagonal One 6 or 6 6 (C6), 6 (C36), 622 (D6) $6mm(C_{6Y}), \frac{6}{m}(C_{6h}),$ Ema (Dah), 6 mm (Dah) Cubic 4 3-fold area 23(T), 432(0), M3 (T_h), T20 (T) M2m $\overline{43m}(T_d), \overline{m3m}(O_b)$

And finally, the cubic point groups the characteristic symmetry is 4 3 fold axes. And we have seen that there are 5 point groups which qualify which has this property of having 4 3 fold axes and they are 2 3 rotation group of tetrahedron 4 32 rotation group of the cube which is also the rotation group of an octahedron Schoenflies uses O for its notation then m 3 bar which is T h and you have complete symmetry of tetrahedron which is 4 bar 3 m Schoenflies notation T d m complete symmetry of the cube m 3 bar m, Schoenflies notation O h.

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So, in this development you can see that the crystal systems are nothing but classification of point groups 32 point groups have been put in these 7 bins based on whether they have these

characteristics symmetry or not. So, crystal system is not really defined by the axial relations, but by the symmetry. So, that point is important.

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4 3-fold axee. 23(T), 432(0), 103 (Th), Cubic $\overline{4}3m(T_{d}), \overline{m3}m(O_{L})$ Crystal Systems are defined by the characteristic symmetry and not by relations between lattice parameters. $a=b=c \quad x=p=3=90^{\circ}$ Crystal Systems are defined by the characteristic symmetry and not by relations between lattice parameters. $\alpha = b = c$ $\alpha = \beta = \vartheta = 90^{\circ}$ Latice parameter relations are satisfied () by the conventional unit cell.

Having said this of course, if the crystal belongs to a particular crystal system one can always select unit cell which satisfies those relations. So, let me take an example. So, a equals b equals c and alpha equal beta equals gamma is equal to 90 degree this is considered to be cubic crystal system, but now, we are seeing that the crystal system is not defined by this relation, but by this relation that crystal system should have 4 3 fold axes or only these five different point groups.

If the crystal has these five point groups, it can be considered as cubic, but once it is considered as cubic, one can select out of many possible unit cells, one can select a unit cell in which this relationship will be satisfied. So, that is what is considered as the conventional unit cell, lattice parameters, lattice parameter relations are satisfied by conventional unit cells. Thank you.